Discussion Materials

Comparison of Alternative PBT Criteria (Organic Chemicals)

Prepared for
PBT Advisory Committee

October 2004

1 Overview

1.1 Purposes of the Discussion Materials

This paper was prepared to provide background information to support discussions by the PBT Advisory Committee. The paper is designed to serve three main purposes:

- Illustrate how policy choices (i.e. choice of criteria for persistence, bioaccumulation, and toxicity) applied within the current technical framework might influence the number and types of chemicals identified as PBT chemicals.
- Describe the technical approaches and information commonly used to characterize the persistence, bioaccumulation potential and toxicity of individual organic chemicals or groups of organic chemicals.
- Highlight some of the important technical choices associated with the use of these technical approaches and available information.

This evaluation builds upon the information and issues discussed at the second meeting of the PBT Advisory Committee held on September 8, 2004. However, the paper is focused on organic chemicals and, consequently, does not address the issues surrounding the evaluation of metals that were identified at that meeting. Ecology is currently reviewing the technical documents prepared by the Environmental Protection Agency on this issue.

1.2 Assumptions Underlying the Discussion Materials

There are several important assumptions that shaped the preparation of this paper. Those assumptions include:

- PBTs are identified on the basis of the intrinsic hazard posed by those chemicals. One of the assumptions underlying this paper is that decisions on whether to include a particular chemical on the PBT list will largely[1] be based on the hazards posed by that chemical. A chemical's hazard is a function of the intrinsic properties of the chemical that relate to persistence, bioaccumulation potential and toxicity. Hazard does not equal risk. An evaluation of risk requires consideration of the hazards associated with a particular chemical and the potential for exposure to that chemical. The potential for exposure is relevant to decisions on priorities and actions to reduce or eliminate uses and releases. (See Figure 1).

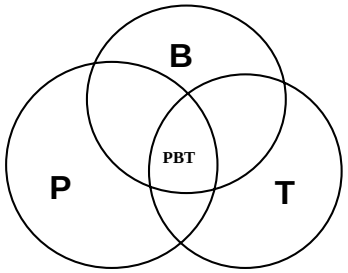
Figure 1

RISK = f (HAZARD x EXPOSURE)

[1] There appeared to be general agreement at the September 8th meeting that Ecology should distinguish between (1) the criteria used to identify PBT chemicals and (2) other factors (independent of the P, B and T characteristics) that are considered when preparing the actual the list. One example of another factor is the Legislative directive to exclude registered pesticides from list.

- The hazard associated with individual chemicals is a function of three chemical characteristics (persistence, bioaccumulation and toxicity). The Legislature directed Ecology to consider the persistence, bioaccumulation potential and toxicity of chemicals when preparing the PBT criteria and list[2]. The Legislative directive is consistent with Ecology's initial decision to focus on those chemicals that display the ability to persist in the environment for long enough periods of time to allow initially low environmental concentrations to increase to toxic levels as the chemical is transferred up the food chain. Ecology believes the chemicals displaying all three characteristics represent a subset of the much larger universe of chemicals that present threats to human and the environment (See Figure 2). However, the decision to focus on chemicals that display all three characteristics should not be interpreted to mean that chemicals that display only two of the characteristics (e.g. persistence and toxic) do not represent significant environmental problems that should be addressed using other regulatory or non-regulatory strategies.

Figure 2
Identifying PBT Chemicals



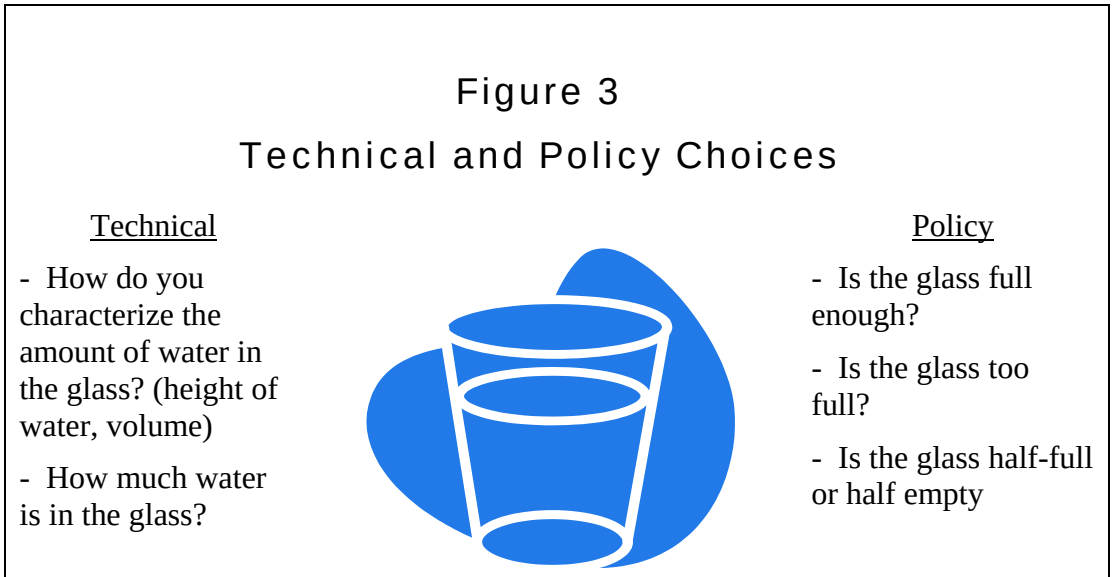
- The comparisons in this paper are based on information for chemicals that have previously been identified as PBT chemicals. Ecology identified an evaluation universe that includes chemicals that have appeared on one or more PBT lists developed over the last 10-15 years. Ecology assumes that the results of such comparisons can provide information that will be useful in selecting from among the alternative criteria suggested by the PBT Advisory Committee at the September 8th meeting.
- Technical approaches and information frame policy choices. This paper also reflects the underlying assumption that decisions on PBT criteria and lists require consideration of a series of scientific/technical and policy issues. The primary focus of this paper is on the scientific and technical choices associated with identifying

[2] This approach is consistent with other national and international programs (See information presented at the August 18th and September 8th PBT Advisory Committee meetings).

parameters to characterize the persistence, bioaccumulation potential and toxicity of individual chemicals and the measures (e.g. reference doses) and measurement scales (e.g. mg/kg/day) for those parameters. Policy considerations drive the selection of fenceline values or criteria that guide decisions on when various measures (e.g. persistence as measured by environmental half-life) are considered high enough (e.g. greater than 2 months) to warrant including a particular chemical on a list of PBTs. Consequently, a secondary objective in preparing this paper was to illustrate how certain policy choices influence the number and types of chemicals that might be included on a PBT list. There are technical and policy choices associated with many types of decisions. For example, there are technical and policy (or value) elements associated with decisions on something as simple as judging the amount of water in glass or cup (See Figure 3). In this simple example, there are a series of technical decisions that need to be made in terms of what is the appropriate parameter to use to characterize how much water is in the glass and how to measure that parameter. The decision on whether the glass is too-full or not-full-enough is a policy choice.

Figure 3

Technical and Policy Choices



- Current toxicology and exposure assessment procedures incorporate reasonable approaches for dealing with the gaps in the current scientific knowledge on the PBT chemicals. The methods for characterizing persistence, bioaccumulation and toxicity incorporate varying degrees of precaution in the face of scientific uncertainty. These methods (e.g. use of uncertainty factors to extrapolate results from animal studies to human populations) have been developed over the last twenty years and continue to evolve as scientists work to better understand the mechanisms underlying various diseases, environmental fate processes, etc. An underlying assumption is that the methods developed over the last ten years by scientific and regulatory organizations incorporate reasonable approaches for dealing with gaps in scientific knowledge.

- The information on persistence, bioaccumulation and toxicity provided in standard databases and reference documents provide a solid technical foundation. The comparisons in this paper are based on information found in readily available databases and information sources. Ecology's confidence in the underlying information is strengthened by the fact that much of the same data has provided the technical foundation for decisions by other organizations over the last 10 years. However, as of October 2004, Ecology has not performed an extensive review of the scientific literature that has appeared in the last two to three years. Ecology anticipates that more detailed reviews of the scientific literature, risk profiles prepared by other organizations etc. will result in some refinement to the conclusions regarding some of the individual chemicals or chemical groups. However, Ecology also believes that such information is unlikely to alter the broad conclusions and relative comparisons in this paper.

1.3 Organization of the Discussion Materials

Section 2 compares various policy options (i.e. choice of criteria for persistence, bioaccumulation, and toxicity) in terms of how those choices might influence the number and types of chemicals identified as PBT chemicals. Descriptions of the technical approaches and information used to characterize the persistence, bioaccumulation potential and toxicity of individual chemicals or chemical groups are included in a series of attachments.

- **Attachment A** summarizes the methods and information used to characterize a chemical's persistence and the range of estimated values for individual chemicals or chemical groups.
- **Attachment B** summarizes the methods and information used to characterize a chemical's bioaccumulation potential and the range of estimated values for individual chemicals or chemical groups.
- **Attachment C** summarizes the methods and information used to characterize a chemical's toxicity (non-cancer health effects) and the range of estimated values for individual chemicals or chemical groups.
- **Attachment D** summarizes the methods and information used to characterize a chemical's carcinogenic potential and the range of estimated values for individual chemicals or chemical groups.
- **Attachment E** summarizes the methods and information used to characterize a chemical's ecological toxicity and the range of estimated values for individual chemicals or chemical groups (Not completed in time for transmittal to Advisory Committee members prior to the October 14th meeting).
- **Attachment F** includes the list of references cited in Sections 1 through 7. (Not completed in time for transmittal to Advisory Committee members prior the October 14th meeting).

2 Comparison of Alternative PBT Criteria

2.1 Purpose of the Comparison

The PBT Advisory Committee discussed a wide range of persistence, bioaccumulation and toxicity criteria that Ecology might use to prepare the PBT list. The alternate approaches suggested by committee members at the September 8th meeting include a range of policy choices on PBT criteria (i.e. what levels of persistence, bioaccumulation, and toxicity are high enough to justify identifying a chemical as a PBT). The purpose of this section is to illustrate how the various policy choices might influence the number and types of chemicals identified as PBTs.

2.2 Methods and Approach

This task was designed to provide a preliminary comparison of alternate policy frameworks for identifying PBTs. It involved the following steps:

- Universe of Chemicals for Comparison ("Comparison List): Ecology reviewed the PBT lists prepared by other organizations over the last 10-15 years and compiled a list of chemicals that have been included on one or more PBT lists. The Comparison List includes 93 individual chemicals or chemical groups (See Table 1). The list includes four metals or organo-metal compounds (cadmium, lead, mercury and tributyltin) and includes some duplication because the list includes both PAHs (the group) and individual PAH compounds (e.g. benzo(a)pyrene).

- Categories or Groups of Chemicals: Ecology condensed the list by lumping together chemicals that share similar characteristics and are commonly considered as chemical groups. For example, the 25-28 individual PAHs that have appear on various lists were combined into a single PAH group. Other groupings include: (1) DDT/DDD/DDE; (2) various forms of hexachlorocyclohexane (e.g. the alpha, beta, delta and gamma forms); (3) chlorinated napthalenes; (4) heptachlor/heptachlor epoxide; (5) endosulfan (alpha and beta forms); (6) chlorinated dibenzo-p-dioxins; and (7) chlorinated dibenzofurans. [**NOTE: At the September 29th PBT Advisory Committee meeting, several committee members expressed concerns about grouping individual chemicals into broad categories. Ecology understands those concerns and is preparing additional comparisons using the full comparison list. Those comparisons will be presented at the October 14th meeting.]**

- Alternate Policy Frameworks: Ecology reviewed the September 8th meeting summary to identify alternative policy frameworks that encompass the different policy choices discussed at that meeting. The four policy frameworks (not listed in any particular order) are:

  - Alternative A: This alternative incorporates the PBT criteria used by Ecology to prepare the PBT Working List:

    - Persistence (regional ½ life > 580 hours);
    - Bioaccumulation (BAF or BCF > 1000);
    - Toxicity (toxicity fencelines described in Attachments C-E).

- Alternative B: This alternative was selected to examine whether there is a significant difference in the number and types of listed chemicals when persistence is characterized using media-specific half life values instead of regional half-life values (Alternative A). The criteria for Alternative B are similar to those used by EPA identify PBT chemicals for reporting under the Toxics Release Inventory Program:
  - Persistence (water ½ life > 2 months or soil ½ life > 2 months);
  - Bioaccumulation (BAF or BCF > 1000);
  - Toxicity (toxicity fencelines described in Attachments C-E).
- Alternative C: This alternative was selected to examine whether there is a significant difference in the number and types of chemicals when persistence is evaluated using a media-specific soil half life value of 6 months instead of 2 months (Alternative B):
  - Persistence (water ½ life > 2 months or soil ½ life > 6 months);
  - Bioaccumulation (BAF or BCF > 1000);
  - Toxicity (toxicity fencelines described in Attachments C-E).
- Alternative D: This alternative was selected to examine whether there is a significant difference in the number and types of chemicals when bioaccumulation potential is evaluated using a BCF or BAF of 5000 instead of 1000 (Alternative C). This alternative is conceptually similar[3] to the criteria specified in the Stockholm Convention.
  - Persistence (water ½ life > 2 months or soil ½ life > 6 months);
  - Bioaccumulation (BAF or BCF > 5000);
  - Toxicity (toxicity fencelines described in Attachments C-E).

- Information Compilation: Ecology compiled available information on persistence, bioaccumulation and toxicity for the chemicals and chemical groups identified in Table 1 using readily available information sources.
- Comparison: Ecology used the information for individual chemicals and chemical groups to compare how many of the 42 chemicals or chemical groups would be included on lists developed using the criteria in Alternatives A through D.

2.3 Preliminary Comparison Results

The comparison results are summarized in Figures 4 and 5. Figure 4 summarizes the comparison results for those chemicals that are not currently registered as pesticides in the United States or Washington. Figure 5 summarizes the comparison results for registered pesticides. **[Ecology does not plan to address the chemicals included in Figure in this rule process because the Legislature directed Ecology not to include registered pesticides on the PBT List. However, the comparison results are included in this handout because the results provide some additional insights on the potential implications associated with the policy choices surrounding the selection of PBT criteria.**] Initial observations include:

[3] This alternative is loosely-based on the criteria reflected in the Stockholm Convention. Differences include: (1) the Stockholm Convention includes separate criteria for long-range transport; (2) the Stockholm Convention includes ½ life criteria for air and sediments; and (3) the Stockholm Convention includes narrative criteria for toxicity.

- The choice of criteria values did not make a large difference in the number of chemicals or chemical groups that would appear on a Washington PBT list. Seventeen (17) chemicals or chemical groups met all four sets of criteria. Five other chemicals met some, but not all of the criteria. (See Figure 4).
- The summary tables masked large differences in the degree to which individual chemicals exceed the various PBT criteria. For example, the bioaccumulation factors/ bioconcentration factors for 4-bromophenyl ether and toxaphene are 1258 and 40,000,000, respectively.
- The sources of information used to characterize the persistence, bioaccumulation potential and toxicity of the chemicals shown in Figure 4 generally fell into the "high" or "highest" data preferences categories identified in WMPT documents. There were some exceptions. For example, the sources of information used to characterize the persistence, bioaccumulation potential and toxicity of the chlorinated napthalenes were generally at the lower end of the data preference hierarchy used by EPA. The differences reflect variations in the attention and studies available for individual chemicals. However, the variations observed in this evaluation were much less than expected. This may be due to the selection criteria used to prepare the Comparison Universe (appearance on one or more PBT Lists) results in a focus on chemicals that have more (rathere than less information).
- The choice of criteria values did make a large difference in the number of registered pesticides meeting the different listing criteria (See Figure 5). Three registered pesticides (hexachlorocyclohexane, isodrin and pentachlorobenzene) met all four sets of criteria. However, use of a higher bioaccumulation criterion (BAF or BCF > 5000) resulted in a much smaller number of registered pesticides meeting the listing criteria. [**NOTE**: The pesticide comparisons are provided for information purposes only. The Legislature specified that registered pesticides should not be included on the PBT list.].
- In contrast to registered pesticides, there was a relatively small (3-5 chemicals or chemical groups) reduction in the number of chemicals that would appear on a Washington PBT list when listing is based on a BAF or BCF value > 5000 (relative to using a BAF or BCF > 1000).
- The number of chemicals identified using media-specific ½ life values is similar to the number of chemicals identified using the EPA Regional ½ life values. Di-n-octyl phthalate was the only chemical identified using the EPA half-life values to characterize persistence that wasn't also included on one or more of the lists developed using media-specific half life values.

2.4 Next Steps

Ecology is currently working to complete a comparison of the four alternatives based on individual chemicals instead of chemical groupings. The results of that comparison will be presented at the October 14th meeting. Ecology also believes it will be important to review and update the underlying technical information based on scientific work completed in the last four years. Beyond those two activities, Ecology believes that additional evaluations or comparisons (if any) will largely depend upon on conversations and feedback from the PBT Advisory Committee, other interested parties and Ecology management.

Figure 4: Comparison Results for Chemicals That Have Appeared On Other PBT Lists (Excluding Registered Pesticides)			
Aldrin			
4-Bromophenyl phenyl ether	Aldrin		
Chlordane	4-Bromophenyl phenyl ether	Aldrin	
Chlordecone (Kepone)	Chlordane	4-Bromophenyl phenyl ether	
DDT p,p', DDD p,p', DDE p, p'	Chlordecone (Kepone)	Chlordane	
Dieldrin	DDT p,p', DDD p,p', DDE p, p'	Chlordecone (Kepone)	Chlordane
Di-n-octyl phthalate	Dieldrin	DDT p,p', DDD p,p', DDE p, p'	Chlordecone (Kepone)
Endrin	Endrin	Dieldrin	DDT p,p', DDD p,p', DDE p, p'
Heptachlor/Heptachlor epoxide	Heptachlor/Heptachlor epoxide	Endrin	Endrin
Hexabromobiphenyl	Hexabromobiphenyl	Heptachlor/Heptachlor epoxide	Heptachlor/Heptachlor epoxide
Hexachlorobenzene	Hexachlorobenzene	Hexabromobiphenyl	Hexabromobiphenyl
Hexchlorobutadiene	Hexchlorobutadiene	Hexachlorobenzene	Hexachlorobenzene
Mirex	Mirex	Hexchlorobutadiene	Hexchlorobutadiene
Octachlorostyrene	Octachlorostyrene	Octachlorostyrene	Octachlorostyrene
Pentabromo diphenyl ether	Pentabromo diphenyl ether	Pentabromo diphenyl ether	Pentabromo diphenyl ether
Polyaromatic hydrocarbons (PAHs)	Polyaromatic hydrocarbons (PAHs)	Polyaromatic hydrocarbons (PAHs)	Polyaromatic hydrocarbons (PAHs)
Polychlorinated biphenyls (PCBs)	Polychlorinated biphenyls (PCBs)	Polychlorinated biphenyls (PCBs)	Polychlorinated biphenyls (PCBs)
Polychlorinated dibenzofurans	Polychlorinated dibenzofurans	Polychlorinated dibenzofurans	Polychlorinated dibenzofurans
Polychlorinated dibenzo-p-dioxins	Polychlorinated dibenzo-p-dioxins	Polychlorinated dibenzo-p-dioxins	Polychlorinated dibenzo-p-dioxins
Polychlorinated napthalenes	Polychlorinated napthalenes	Polychlorinated napthalenes	Polychlorinated napthalenes
Tetrabromobisphenol	Tetrabromobisphenol	Tetrabromobisphenol	Tetrabromobisphenol
Toxaphene	Toxaphene	Toxaphene	Toxaphene
Alternative A	**Alternative B**	**Alternative C**	**Alternative D**

Figure 5 – Comparison Results for Registered Pesticides That Have Appeared On Other PBT Lists (Information Only)			
Endosulfan			
Hexachlorocyclohexane (Lindane)	**Hexachlorocyclohexane (Lindane)**		
Isodrin	**Isodrin**	**Hexachlorocyclohexane (Lindane)**	
Methoxychlor	**Methoxychlor**	**Isodrin**	
Pendimethalin	**Pendimethalin**	**Pendimethalin**	
Pentachlorobenzene	**Pentachlorobenzene**	**Pentachlorobenzene**	
Pentachloronitrobenzene	**Pentachloronitrobenzene**	**Pentachloronitrobenzene**	
1,2,3,4-Tetrachlorobenzene	**1,2,3,4-Tetrachlorobenzene**	**1,2,3,4-Tetrachlorobenzene**	
1,2,4,5-Tetrachlorobenzene	**1,2,4,5-Tetrachlorobenzene**	**1,2,4,5-Tetrachlorobenzene**	**Hexachlorocyclohexane (Lindane)**
1,2,4-Trichlorobenzene	**1,2,4-Trichlorobenzene**	**1,2,4-Trichlorobenzene**	**Isodrin**
Trifluralin	**Trifluralin**	**Trifluralin**	**Pentachlorobenzene**
Alternative A	**Alternative B**	**Alternative C**	**Alternative D**

Table 1: Universe of Chemicals Included in Comparative Analysis

Chemical	CAS	ARET	Great Lakes - Level 1 Substances	Great Lakes - Level 2 Substances	EPA National Strategy	EPA - Toxics Release Inventory	EPA Waste Minimization (30)	UNEP - POPS	Commission of the European Communities (April 2004 Proposal)
DDT p, p'-	50293		X		X			X	
Benzo(a)pyrene	50328	X	X			X			
Dibenzo(a,h)anthracene	53703	X				X			
Tributyltin (oxide)	56359	X							
3-Methylcholanthrene	56495					X			
Benzo(a)anthracene	56553	X				X			
Chlordane	57749		X		X	X		X	
7,12-Dimethylbenz(a)anthracene	57976					X			
Hexachlorocyclohexane (g) (Lindane)	58899	X		X			X		X
Dieldrin	60571		X		X			X	
Hexachloroethane	67721						X		
Endrin	72208			X				X	
Methoxychlor	72435					X	X		
DDD p,p'-	72548		X		X			X	
DDE p,p'-	72559		X		X			X	
Heptachlor	76448			X		X	X	X	
Tetrabromobisphenol A	79947					X			
Pentachloronitrobenzene	82688						X		
Acenapthene	83329						X		
Phenanthrene	85018	X					X		
Fluorene	86737						X		
Hexachlorobutadiene	87683			X			X		X

Chemical	CAS	ARET	Great Lakes - Level 1 Substances	Great Lakes - Level 2 Substances	EPA National Strategy	EPA - Toxics Release Inventory	EPA Waste Minimization (30)	UNEP - POPS	Commission of the European Communities (April 2004 Proposal)
Pentachlorophenol	87865	X		X			X		
3,3'-dichlorobenzidine	91941			X					
1,2,4,5-Tetrachlorobenzene	95943			X			X		
2,4,5-Trichlorophenol	95954						X		
4'4-Methylenebis(2-chloroaniline)	101144	X		X					
4-Bromophenyl phenyl ether	101553						X		
1,4 Dichlorobenzene	106467			X					
Bis(2-ethyl-hexyl)phthalate	117817								X
Di-n-octyl phthalate	117840								X
Hexachlorobenzene (HCB)	118741	X	X		X	X	X	X	
Anthracene	120127						X		
1,2,4-Trichlorobenzene	120821						X		
Pyrene	129000	X					X		
Chlordecone (Kepone)	145500								X
Benzo(r,s,t)pentaphene	189559					X			
Dibenzo (a,h)pyrene	189644					X			
Benzo(g,h,i)perylene	191242	X				X	X		
Dibenzo (a,l)pyrene	191300	X				X			
Dibenzo (a,e)pyrene	192654					X			
Indeno(1,2,3-cd)pyrene	193395	X				X			
7H-Dibenzo(c,g)carazole	194592					X			
Perylene	198550	X	X						
Benzo(j)fluoranthene	205823	X				X			
Benzo(b)fluoranthene	205992	X				X			
Fluoranthene	206440	X				X			
Benzo(k)fluoranthene	207089	X				X			
Acenaphthylene	208968						X		
Benzo(a)phenanthrene	218019					X			

Chemical	CAS	ARET	Great Lakes - Level 1 Substances	Great Lakes - Level 2 Substances	EPA National Strategy	EPA - Toxics Release Inventory	EPA Waste Minimization (30)	UNEP - POPS	Commission of the European Communities (April 2004 Proposal)
Dibenzo(a,j)acridine	224420	X				X			
Dibenzo(a,h)acridine	226368					X			
Aldrin	309002		X		X	X		X	
Hexachlorocyclohexane (a)	319846	X		X					
Hexachlorocyclohexane (b)	319857			X					
Hexachlorocyclohexane (d)	319868			X					
Isodrin	465736					X			
Pentachlorobenzene	608935			X		X	X		
1,2,3,4-Tetrachlorobenzene	634662			X					
Endosulfan (alpha)	959988						X		
Heptachlor epoxide	1024573				X				
Pentachloronapthalene	1321648								X
Trichloronapthalene	1321659								X
Hexachloronapthalene	1335871								X
Tetrachloronapthalene	1335882								X
Polychlorinated biphenyls	1336363	X	X		X	X	X	X	
Trifluralin	1582098					X	X		
2,3,7,8 TCDD	1746016	X	X		X	X	X	X	
Mirex	2385855		X		X			X	
Octachlorodibenzo-p-dioxin	3268879					X			
5-Methylchrysene	3697243					X			
Dibenzo(a,e)fluoranthene	5385751					X			
1-Nitropyrene	5522430					X			
Lead	7439921		X		X		X		
Mercury	7439976	X				X	X		
Cadmium	7440439			X			X		
Toxaphene	8001352		X		X	X			
Octachlorostyrene	29082744	X	X		X	X			

Chemical	CAS	ARET	Great Lakes - Level 1 Substances	Great Lakes - Level 2 Substances	EPA National Strategy	EPA - Toxics Release Inventory	EPA Waste Minimization (30)	UNEP - POPS	Commission of the European Communities (April 2004 Proposal)
Pentachlordibenzofuran	30402154					X			
Heptachloronapthalene	32241080								X
Pentabromo phenyl ether	32534819								X
Endosulfan (beta)	33213659						X		
Hexachlorodibenzo-p-dioxin	34465468					X			
Pentachlorodibenzo-p-dioxin	36088229					X			
Hexabromobiphenyl	36355018								X
Heptachlorodibenzo-p-dioxin	37871004					X			
Heptachlordibenzofuran	38998753					X			
Octachlorodibenzofuran	39001020					X			
Pendimethalin	40487421					X	X		
2,3,7,8 Tetrachlorodibenzofuran	51207319					X			
Hexachlorodibenzofuran	55684941					X			
Dinitropyrene	78432196	X		X					
Polyaromatic hydrocarbons (PAHs)		X	X		X	X	X		